11-FEB-76 11:04:00-PST,4172;000000000000
Date: 11 FEB 1976 1104-PST
From: WIPKE
Subject: Details of Resource Related Proposal
To: Lederberg
cc: wipke

        Here are some details on the proposal. I will call you

late this afternoon or Thursday morning to get any feedback.
If there is anything else I should include, please
let me know.

EQUIPMENT
        2 leased lines to SUMEX including modems (total $4500)
        Memory expansion of GT40
        Interface to 9 trk tape drive
        3-D tablet and interface to GT40
        Printer/plotter and interface to GT40
        Floppy disk so can run RT11 operating system on GT40
        16 mm movie camera

SUPPLIES
        Manuals and documents ($500)
        Various other paper supplies and tapes for local equipment.
        additional terminals (2) Texas Instruments or TV type.

PERSONNEL
        2 Graduate Students
        3 Postdoctoral STudents
        1 Secretary (manuscripts and documentation and interfacing
                with remote users)

RESEARCH TO BE COVERED
        Development of computer assisted design of organic synthesis
                complete coverage of reaction types in data base
                strategy development for multistep synthesis using
                        stereochemistry and steric information
                long term planning for multistep synthesis
                Block avoidance in synthesis by subgoals
                More accurate evaluation of reactions based on
                        3-d models, and other chemical info
                Availability of production synthesis program to
                        synthesis community.
                Support of production synthesis program, handling user
                        comments and problems.
        Development of forward working synthels program to complement
                the backward planning program.
                Accurate prediction of chemical reactions based on
                        constitution and 3-D structure
                3-D Molecular model building, display, manipulation,
                        and evaluation.
                3-D pattern matching (biomolecular patterns)
        Development of computer graphics in biomolecular applications.

RATIONALE
        Organic synthesis is extremely important to the health community
for it provides new drugs, test molecules, and modifications to natural
materials. NIH supports many synthetic chemists to synthesize new
compounds of interest to them or just to develop new methodology in
organic synthesis. The computer synthels program will be able to
provide a useful consulting service to these chemists. In additon,
many new algorithms have been developed in this research which are use-
ful to all other research in computer applications to chemistry,
biochemistry, etc.

        The DENDRAL project deals largely with structure elucidation
whereas the SECS project deals largely with molecular construction.
Although they are different in most respects, they both have to

represent molecular structures, interface to chemists, and
sometimes even use similar algorithms, for example to recognize
when two structures are equivalent.

The interaction of the two projects allows transfer of
experience in different areas efficiently. We have had joint group
meetings monthly and at least from my group's point, they have been
stimulating and we would very much like to continue the interaction.

WHAT NEXT?
After we discuss this on the phone, we need to put
together a one page summary of
1. What I will provide
2. What SUMEX will provide
3. Indicate to NIH that it is advantageous to SUMEX and
to my project that there be a RESOURCE RELATED
proposal and that there be interaction.

Regarding file space, we do need probably eventually more than we
now have. I hope that by having a mag tape locally here, we can
not have to keep all our files on-line which is wasteful and unnecessary
since we do not work on all of them every day or even every week.
I don't know how much a disk for your system would cost,
but it might be possible to put that in my proposal. I only worry
that increasing my budget too much may decrease my chances of approval.
I have been without a grant to support my computer work all this year
and am having to support a number of students here by consuming equipment
money that the department allocated to me etc, so I desparately
need to assure that this grant is approved. But I would be happy
to do whatever would help SUMEX.